



**Figure** : MCML and mcxyz comparison on a 2-layer skin tissue(layer1: 60um-thick epidermis; layer2:840um-thick dermis). (A) shows the tissue types and the photon path(in green lines). (B) shows the attenuation of the axial fluence  $F_{zx}$  through the fiber tip. The maximum difference occurs at the fiber tip, which is ~10% difference and the difference quickly reduces as the distance from the fiber tip increases. After the distance from the tip reaches ~120um, the mcml and mcxyz have essentially identical output for both flat beam and Gaussian beam. The difference is due to different tissue boundary approaches. In the optogenetical simulation, when the fiber is implanted into the brain tissue, the effect of the boundary conditions would not be significant.

**Simulation parameters:** collimated flat beam or Gaussian beam at 532nm is delivered to the top of epidermis through an optical fiber with a core diameter of 200um. 650,000 photons were launched in MCML, while 2-minutes simulation time was set in mcxyz, launching about ~650,000 photons. For layer 1:  $n = 1.37$ ,  $ua=16.5724\text{cm}^{-1}$ ,  $us=375.9\text{cm}^{-1}$ ,  $g = 0.9$  ; For layer2:  $n = 1.37$ ,  $ua=0.4585\text{cm}^{-1}$ ,  $us=365.5\text{cm}^{-1}$ ,  $g = 0.9$  . The top medium optical properties is set to:  $n = 1.37$ ,  $ua=0.1\text{cm}^{-1}$ ,  $us=10\text{cm}^{-1}$ ,  $g = 0.9$ .